AAPG Annual Convention
Salt Lake City, Utah
May 11-14, 2003

Evaluation of hydrologic and biogeochemical controls on soluble benzene migration within the Uinta Basin using computer models and field sampling

Ye Zhang, Department of Geological Sciences, Indiana University, Bloomington, IN; Mark A. Person, Department of Geological Sciences, Indiana University, Bloomington, IN; Enrique Merino, Department of Geological Sciences, Indiana University, Bloomington, IN; Michael Szpakiewcz, Fossil Energy Technologies, Idaho National Engineering and Environmental Laboratory, Idaho Falls, ID

Introduction

In this study, benzene was analyzed from oil and brine samples taken from the Uinta Basin. Springs hydraulically down gradient from the oil fields were also sampled. Using a mathematical model of groundwater flow, heat transfer and coupled solute mass transport within the basin and an oil reservoir, we have been able to quantitatively assess the effects of groundwater flow and microbial processes on the transport and attenuation of benzene in sedimentary basins.

The occurrences of BTEX as dissolved solutes in oil field brines and as soil gases near known oil fields have led some to promote BTEX compounds as a geochemical exploration tool for petroleum. Among BTEX compounds, benzene is found in oil with concentrations up to 19,298 ppm and in oil field brines with concentrations up to 17.7 ppm. Elevated benzene concentrations have been reported in formation groundwater up to 22 km from oil fields. However, as distance from an oil field increases, benzene content in groundwater diminishes. Prior studies have proposed aqueous diffusion as the dominant mechanism for BTEX transport. To explain BTEX soil gas anomalies, separate phase microseepage from oil reservoirs as gas bubbles was proposed. However, benzene and toluene have also been found within the groundwater discharge areas of east-central Alberta, not directly over any oil fields. BTEX thermodynamic phase diagrams indicate that these compounds exist as a liquid under the subsurface temperature and pressure conditions that characterize sedimentary basins (Fig. 1). Microseepage of BTEX as gas bubbles appears unlikely. BTEX compounds also attenuate naturally in the subsurface due to biodegradation (Fig. 2). Among BTEX compounds, benzene is the most soluble, least sorptive and most resistant to anaerobic biodegradation. It thus persists in groundwater the longest and has become the focus of our study.

Mathematical model

The mathematical model we developed solves coupled steady-state groundwater flow and heat transfer equations (Fig. 3). The calculated hydraulic heads, groundwater flow rates and temperatures are in turn used by a transient solute transport model which solves the advective/dispersive benzene transport in the basin and its diffusive transport within an oil reservoir. Benzene attenuation is represented using biodegradation rates estimated for shallow groundwater flow systems. The two transport models are coupled at the oil-water contact where equilibrium partitioning of benzene from the oil phase to the aqueous phase is assumed. A thermodynamic model was used to calculate the equilibrium constant under reservoir temperature and pressure conditions (Fig. 4). Details of the model can be found in Zhang et al. (in press).

To interpret existing field data of benzene found in formation brines from a variety of basins, a simple, idealized model was first constructed to represent benzene transport in a carrier bed adjacent to an oil reservoir. Both diffusion and advection dominated systems were represented. Advection/dispersion model modified by biodegradation can create the decay of the benzene concentration profiles that fall within the range of field data after a few million years of transport. Diffusion model requires a transport time scale in excess of 1 billion years to migrate the average observed distance of 10 km (Fig. 5).

The Uinta Basin

The Uinta Basin in Utah contains a number of well documented oil fields, an active regional groundwater flow system and high quality geologic data sets (Fig. 6). Numerous bitumen-bearing sandstone deposits are found along the southern edge of the basin (e.g. north of Book Cliffs), indicating that biodegradation and water washing of the oils has occurred. A northwest-south geological transect across the basin and two oil fields was constructed, following the general direction of the regional groundwater flow (Fig. 7). The transect extends from the Uinta Mountains in the north to the south of the Books Cliff with a total length of 142 km and a maximum thickness of 8800m. Major stratigraphy represented by the cross section includes the Mesaverde Group, the North Horn Formation, the Colton Formation, the Wasatch Formation, the Green River Formation, the Duchesne-Uinta Formations, and the Uinta Mountain Formation. Thin layers of Paleozoic and Mesozoic rocks were thrust upwards along the South Flank Fault in between the Wasatch Formation and the Uinta Mountain Formation. There rocks are generally permeable and act as fluid conduits for the deep basin. Below the Mesaverde Group is the Mancos shale which is assumed in this study to constitute an impermeable base of the model.

There distinct groundwater flow systems exist within the Uinta Basin (Fig. 8). Within the Duchesne and Uinta Formations and the upper Green River Formation, groundwater is driven by the topographic relief of the Uinta Mountains and is normally pressured. Within the lower Green River Formation at the Altamont-Bluebell field, groundwater is over-pressured due to oil generation. Within the basal Mesaverde Group, groundwater is sub-hydrostatic. The groundwater flow rates within the upper flow system of the Duchesne-Uinta Formations are high enough to disturb the subsurface thermal regime (Fig. 9). Negative temperature anomalies in excess of 20°C have been observed adjacent to the Uinta Mountains, corresponding to the regional groundwater recharge area. Positive thermal anomalies have been observed near the groundwater discharge area.

Field Sampling

Benzene was sampled from oils and brines of the Altamont-Bluebell and Pariette Bench fields in the Uinta Basin and was also sampled from springs and seeps down hydraulic gradient from these oil fields. The concentrations were measured using gas chromatography. The average benzene concentrations in oils and co-produced brines are 1946 and 4.9ppm at the Altamont-Bluebell field and 1533 and 0.6ppm at the Pariette Bench field, respectively. Benzene was below the detection limit in all the springs sampled.

Model application in Uinta Basin

The transport equations were solved numerically using a triangular finite element discretization of the basin and the oil reservoir domains (Fig. 10). Permeability and porosity of the lithological units were assigned based on published data and varied in a model calibration exercise. Fluid flow and heat transfer was calibrated using the observed pressure and temperature conditions (Fig. 11). Soluble benzene transport from the over-pressured Altamont-Bluebell field was represented after 5 million years in the coupled basin/reservoir system, with and without representing bacterial attenuation (Fig. 12). Without representing attenuation, results of benzene transport indicate that benzene partitions out of the oil phase at the oil-water contact and is transported away from the reservoir by groundwater via advection to the water table. A sizable geochemical plume formed along the transport path and dissolved benzene in groundwater reaches the discharge area in about 1 million years. After 5 million years, significant concentrations of benzene occur at the groundwater outflow areas of the central river valley, almost directly overlying the oil field. On the other hand, the attenuation model predicts that benzene is closely contained near the oil deposit (within 4km) and is not able to reach the surface, consistent with the sampling results from springs. Attenuation has also significantly modified the shape of the dissolved benzene plume to be ring-like, analogous to that of a diffusion dominated system. The advective nature of the transport (Fig. 12a) has been totally masked. More waterwashing within the oil reservoir has also occurred through time.

Discussion

Our results suggest that soluble BTEX transport in basins is dominated by advection and modified by bacterial attenuation. The average observed aqueous BTEX migration distance shown in Fig. 5 (approximately 10 km) can not be explained by diffusion because the time required for diffusional transport exceeds the age of the basins sampled. Advective transport of BTEX by groundwater can form extensive subsurface geochemical anomalies surrounding an oil field. Biodegradation can significantly modify the shape and the distance of soluble BTEX transport down-gradient from an oil reservoir and determine whether these compounds can be found in measurable concentrations in springs. Results of the Uinta Basin models indicate that benzene attenuation must have occurred along the transport path in this basin since models representing attenuation predicted results consistent with the field measurements. However, in the case of finding BTEX at the groundwater discharge areas of the Alberta Basin, it's probably the result of advective transport by groundwater from an oil deposit which lies nearby with a direct hydraulic connection to the springs.

Advective transport of BTEX by groundwater can also form surface geochemical anomalies, sometimes near the edge of the oil fields ("edge" phenomena). Excluding contamination from fuel spills, soil BTEX gas anomalies most likely result from volatization at the water table during the final stage of their migration, either as dissolved solutes in groundwater or as separate phase oil through large continuous fractures. In the case of their buoyancy-driven separate phase migration via fractures, a threshold aperture size of about1.0 mm or larger is required for BTEX to reach the surface before diffusing out of the oil into the formation water. Surface geochemical exploration based on BTEX soil gas anomalies can be effective only after the mechanism as well as the entire migration pathway has been delineated.

Conclusion

BTEX detected in exploration wells may provide a useful indicator of a nearby oil reservoir. However, the effects of hydrodynamics on BTEX transport should be considered. Based on existing data, this distance is generally on the order of several kilometers or higher. Chemical sampling of BTEX in springs can be effective only when the oil reservoir is located close-by (within 22 km - the maximum observed distance of dissolved benzene in formation water from an oil field). In most basins, subsurface biodegradation processes reduce the BTEX concentration below the detection limit at transport distances much shorter (within 10 km). Unless large continuous fracture network exist between the oil reservoir and the land surface, BTEX soil gas anomalies may be controlled by regional hydrodynamics rather than by separate phase migration. Subsurface temperature anomalies can also form in association with the geochemical anomalies and can indicate the direction of groundwater flow. Knowledge of these hydrological, thermal and biogeochemical conditions in a basin should help in the better interpretation of BTEX surface and subsurface anomalies.

Future research

BTEX biodegradation rate data is badly needed at the temperature, pressure and salinity conditions consistent with oil reservoirs. Laboratory column experiments should be conducted under in-situ conditions using microbes extracted from strata near oil reservoirs. Comparison of BTEX migration in oil-bearing marine basins and terrestrial basins would shed light on the differences as well as similarities of BTEX migration within these two systems.

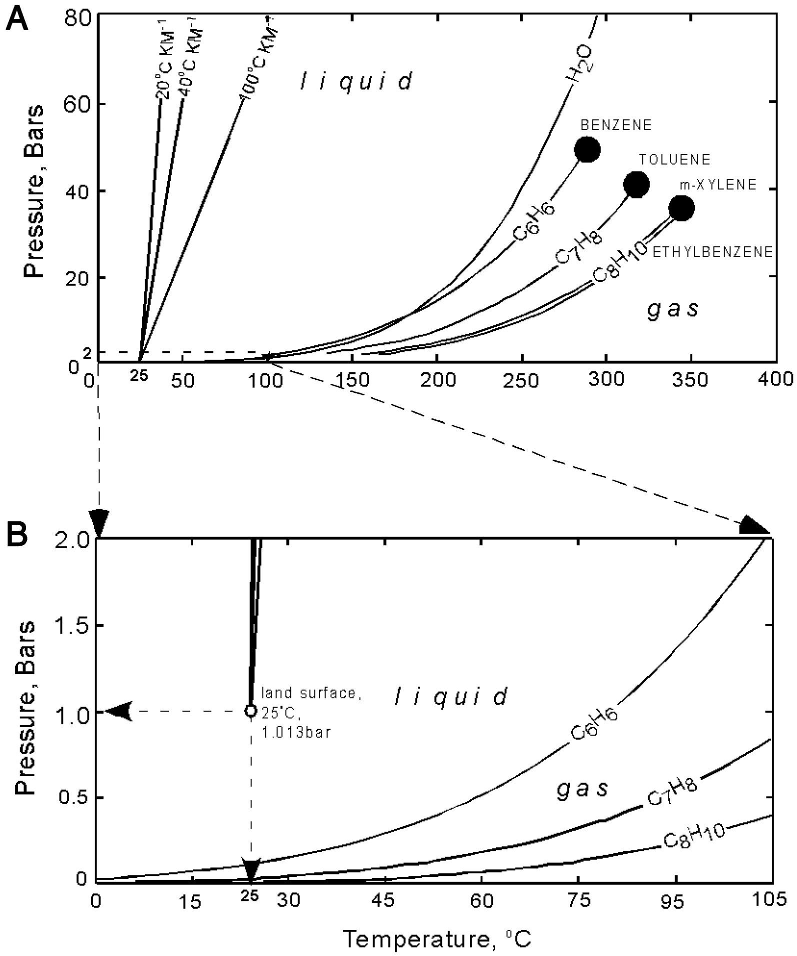


Figure 1. (A) BTEX and water boiling curves and critical points (dots) (from Helgeson, et al., 1998). (B) BTEX boiling curves at the near-surface to surface temperature and pressure conditions (Aljoe et al., 1986). Three representative geotherms of sedimentary basins are superimposed onto each plot. The geotherms do not intersect with the BTEX boiling curves, indicating that these compounds exist as a liquid under the typical subsurface (reservoir) temperature and pressure conditions.

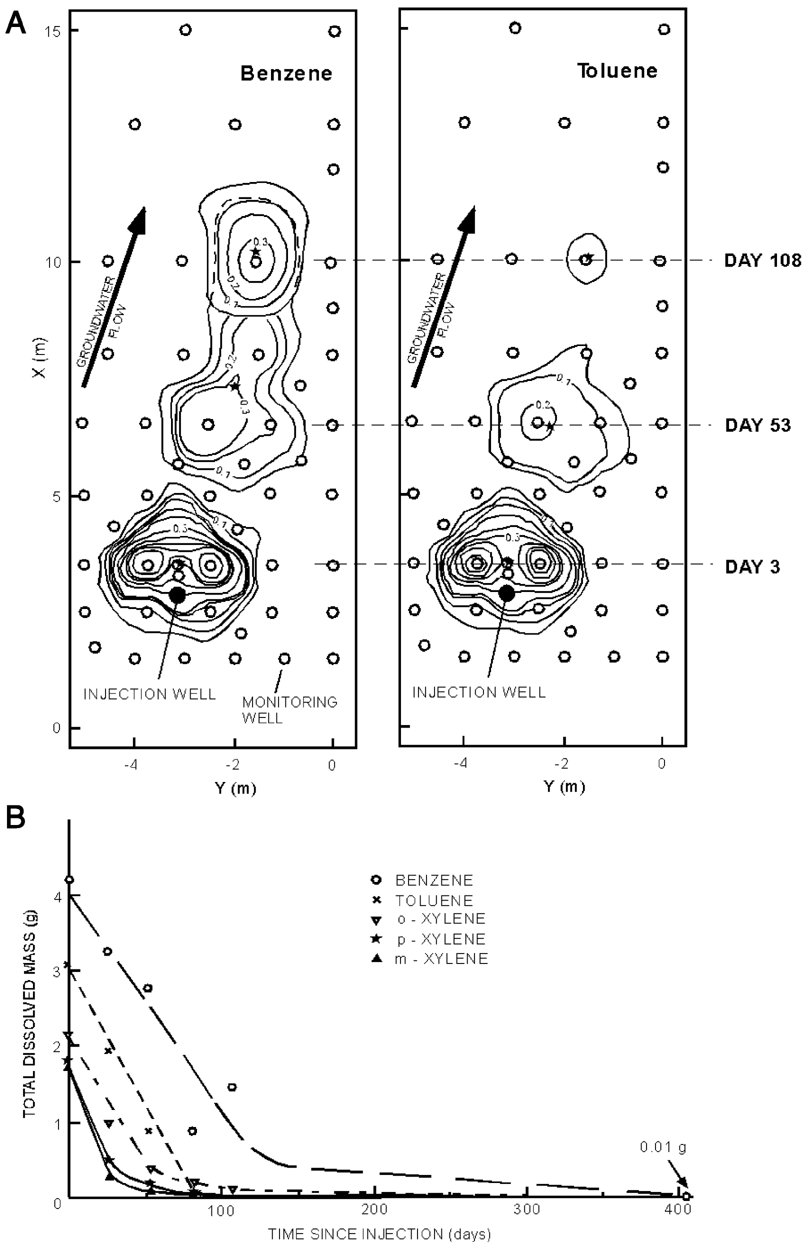


Figure 2. (A) Plan views of benzene and toluene concentration contours (depth-averaged; in µg/m^2) on day 3, 53 and 108 in a natural gradient injection experiment at Canada Force's Base, Borden, Ontariao (from Barker et al., 1989). Stars represent the center of mass for the plume evolution over time. (B) The change of the total dissolved solute mass of benzene, toluene and xylene in groundwater over 410 days of experiment (from Barker et al., 1989). Aerobic biodegradation was proposed as the main mechanism for their mass loss. Among BTEX compounds, benzene in groundwater persists the longest over time.

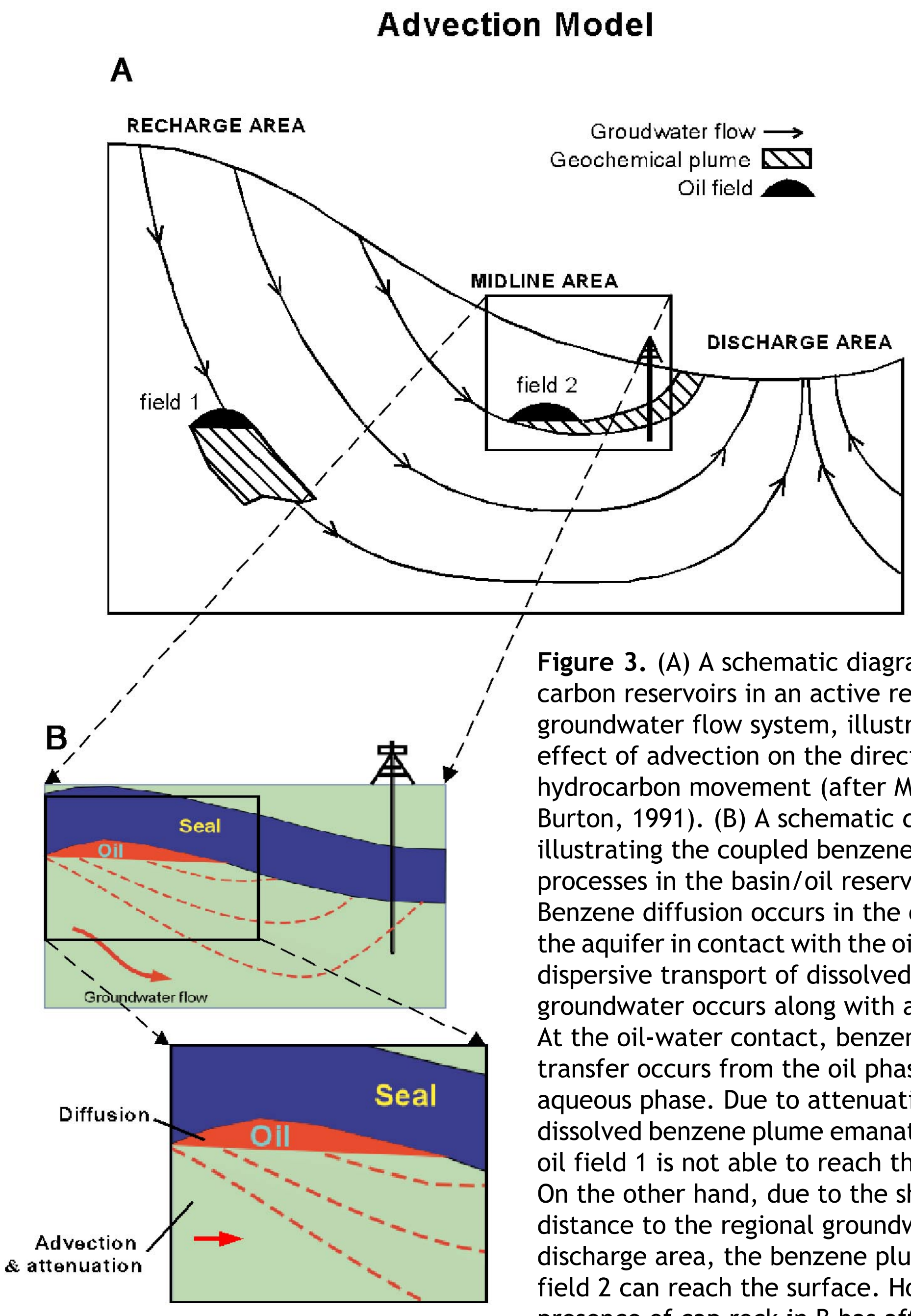


Figure 3. (A) A schematic diagram of hydrocarbon reservoirs in an active regional groundwater flow system, illustrating the effect of advection on the direction of hydrocarbon movement (after Machel and Burton, 1991). (B) A schematic diagram illustrating the coupled benzene transport processes in the basin/oil reservoir system. Benzene diffusion occurs in the oil, while in the aquifer in contact with the oil, advective-dispersive transport of dissolved benzene by groundwater occurs along with attenuation. At the oil-water contact, benzene mass transfer occurs from the oil phase to the aqueous phase. Due to attenuation, the dissolved benzene plume emanating from the oil field 1 is not able to reach the surface. On the other hand, due to the shorter distance to the regional groundwater discharge area, the benzene plume from oil field 2 can reach the surface. However, the presence of cap rock in B has affected the direction of the solute plume migration.

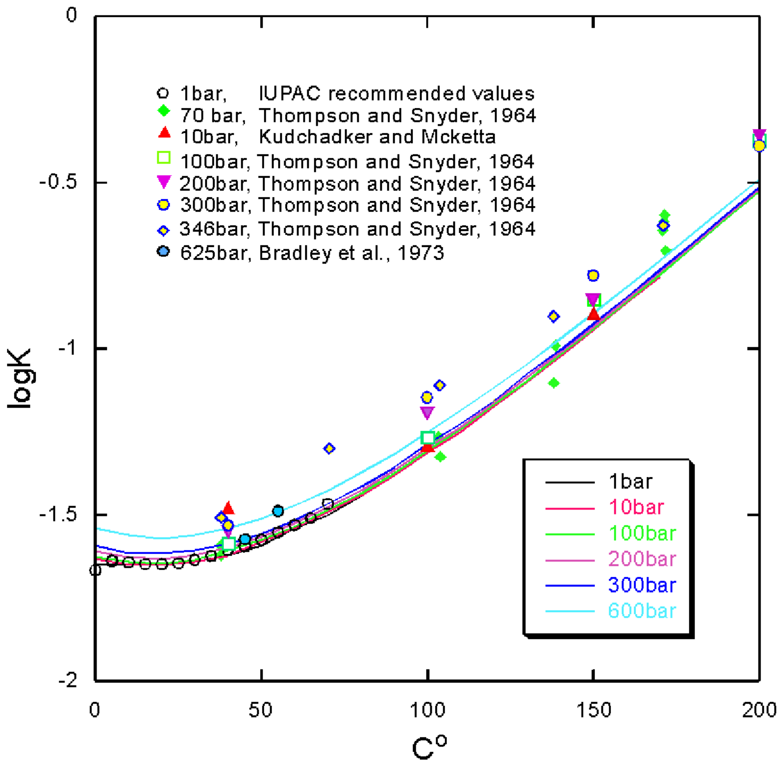


Figure 4. Theoretical predictions of equilibrium constant (logK in curves) for the benzene dissolution reaction, calculated using SUPCRT92 and the thermodynamic properties of liquid and aqueous benzene (Johnson et al., 1992; Shock and Helgeson, 1990; Richard and Helgeson, 1998). Superimposed are experimental solubilities (dots) of benzene in water measured under different temperature and pressure conditions (all referenced works are listed in the IUPAC solubility data series, 1989). The theoretical predictions fit the experimental solubility data well within 1 log unit and is considered a good fit.

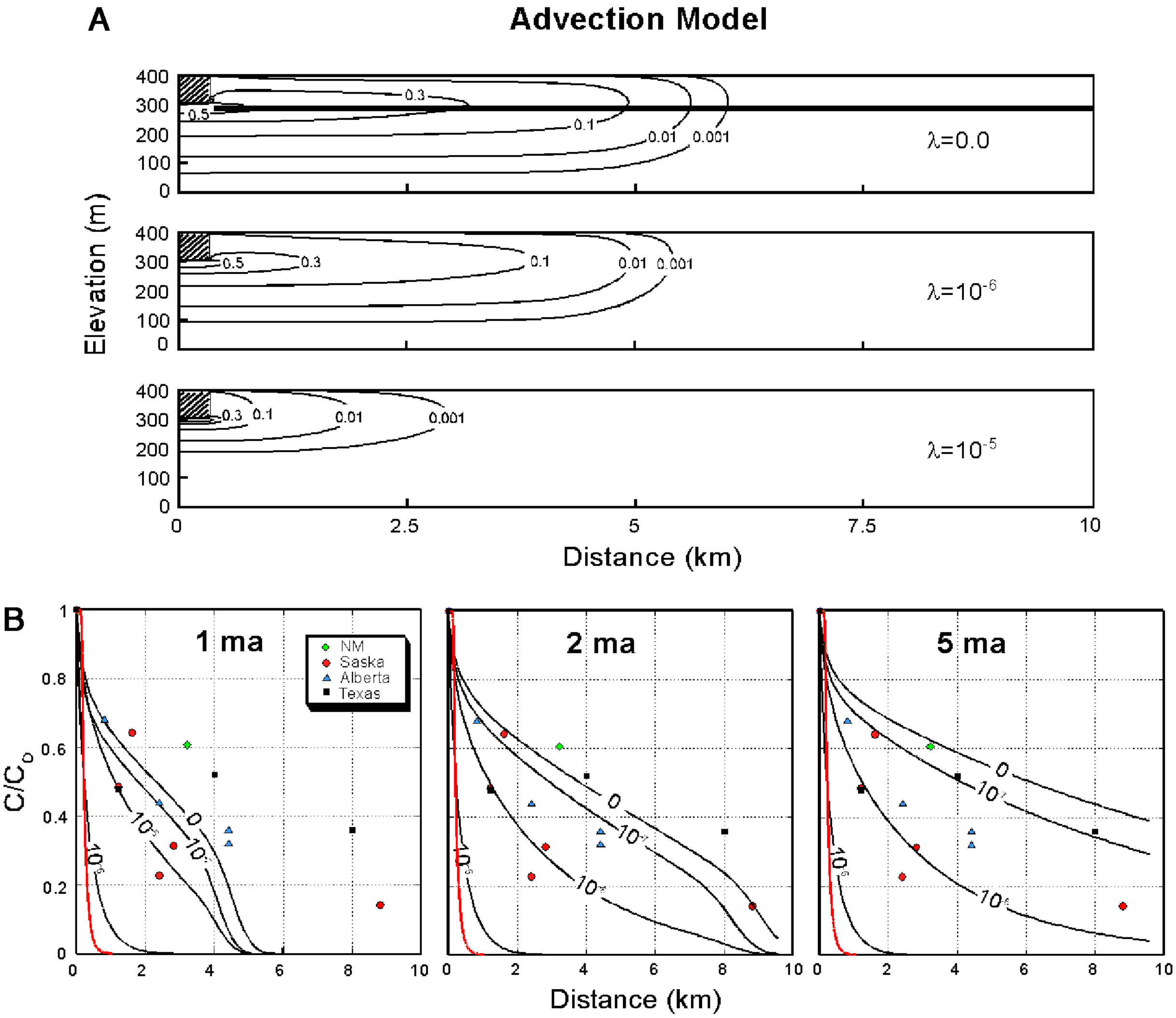


Figure 5. (A) Benzene concentrations (in ppm - black lines) in the carrier bed after 1 million years of advective/dispersive transport. Groundwater velocity within the carrier bed is about 0.005 m/yr. A model without biodegradation (λ=0.0 yr^{-1}) and models representing two different rates of biodegradation ($\lambda=10^{-6}$, $\lambda=10^{-5}$) are shown. (B) Concentration profiles of benzene sampled along a single horizon within the carrier bed down hydraulic gradient from the oil reservoir (bold line in A). The profiles include different rates of biodegradation at different simulation time. The numbers on the lines refer to the biodegradation rate used. 0 represents no biodegradation and 10^{-5} represents a biodegradation rate three orders of magnitude lower than those measured in shallow groundwater systems. Field data (Zarrella et al., 1967) as well as the profile calculated by the diffusion model (red lines) after 100 million years of transport are plotted for comparison. The magnitude of the effective diffusion coefficient is on the order of 10^{-11} m^2/s.

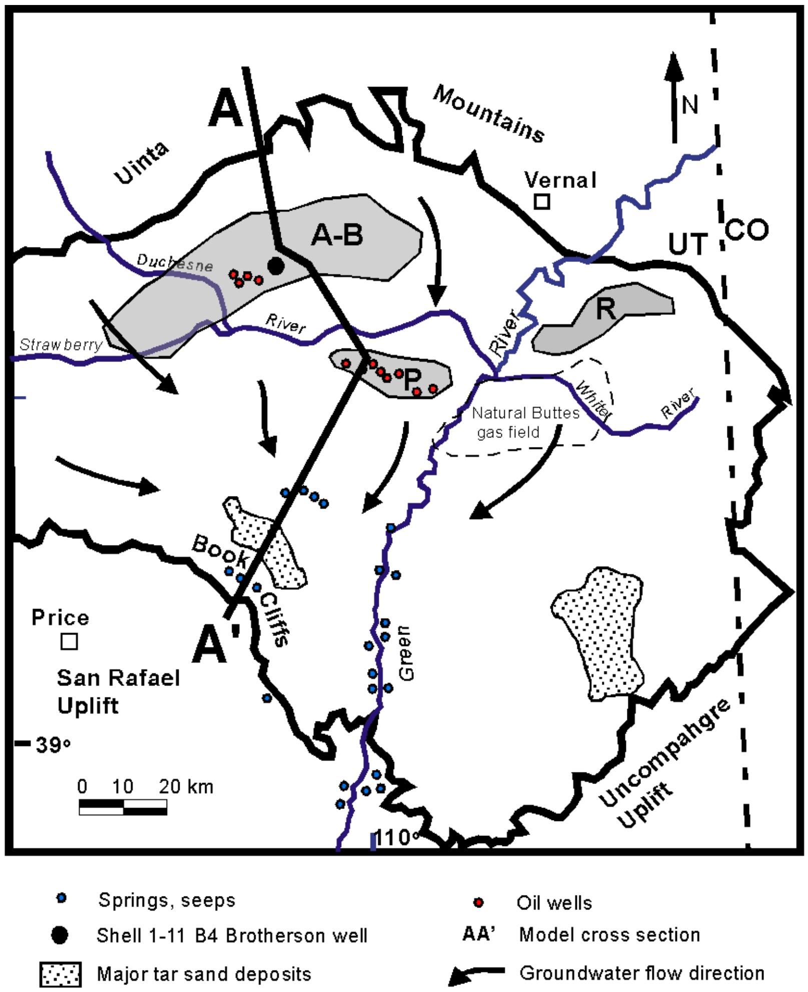


Figure 6. The Uinta Basin with the location of the major oil fields (A-B: Altamont-Bluebell; R: Redwash; P: Pariette Bench), the model cross section (A-A´), and the location of the major tar sand deposits (after Bredehoeft et al., 1994). Also shown is the location of the field samples collected for this study. Based on the potentiometric surfaces of the basin stratigraphy, generalized direction of regional groundwater flow is indicated by the long arrows.

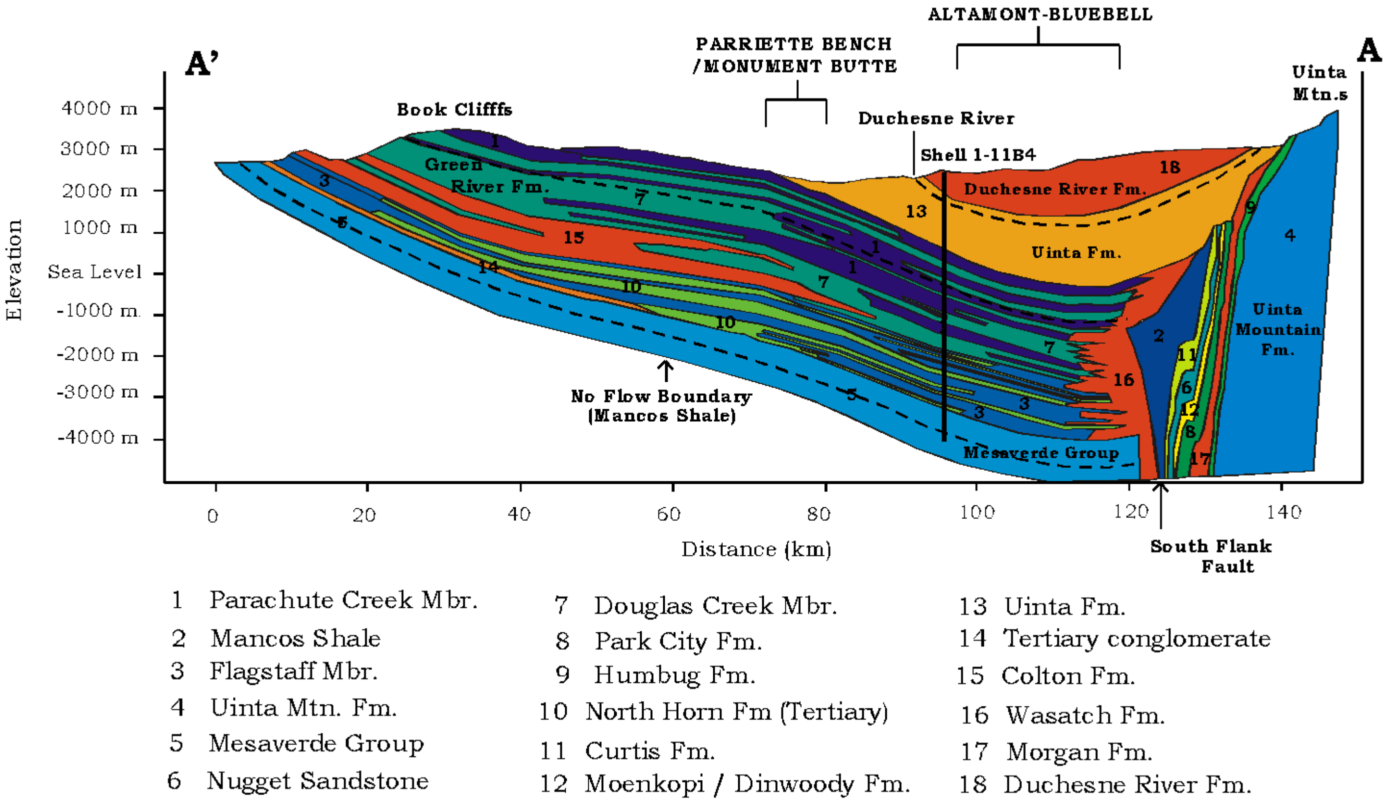


Figure 7. The lithostratigraphic units represented by the cross section AA´(after Fouch, 1975; Pitman, et al., 1982; Bredehoeft et al., 1994). The locations of Uinta Mountains, Book Cliffs and Duchesne River are indicated along with Shell 1-11 B4 well projected onto the cross section. Three dashed lines are the depths at which heads calculated by the numerical models are calibrated against the observed heads.

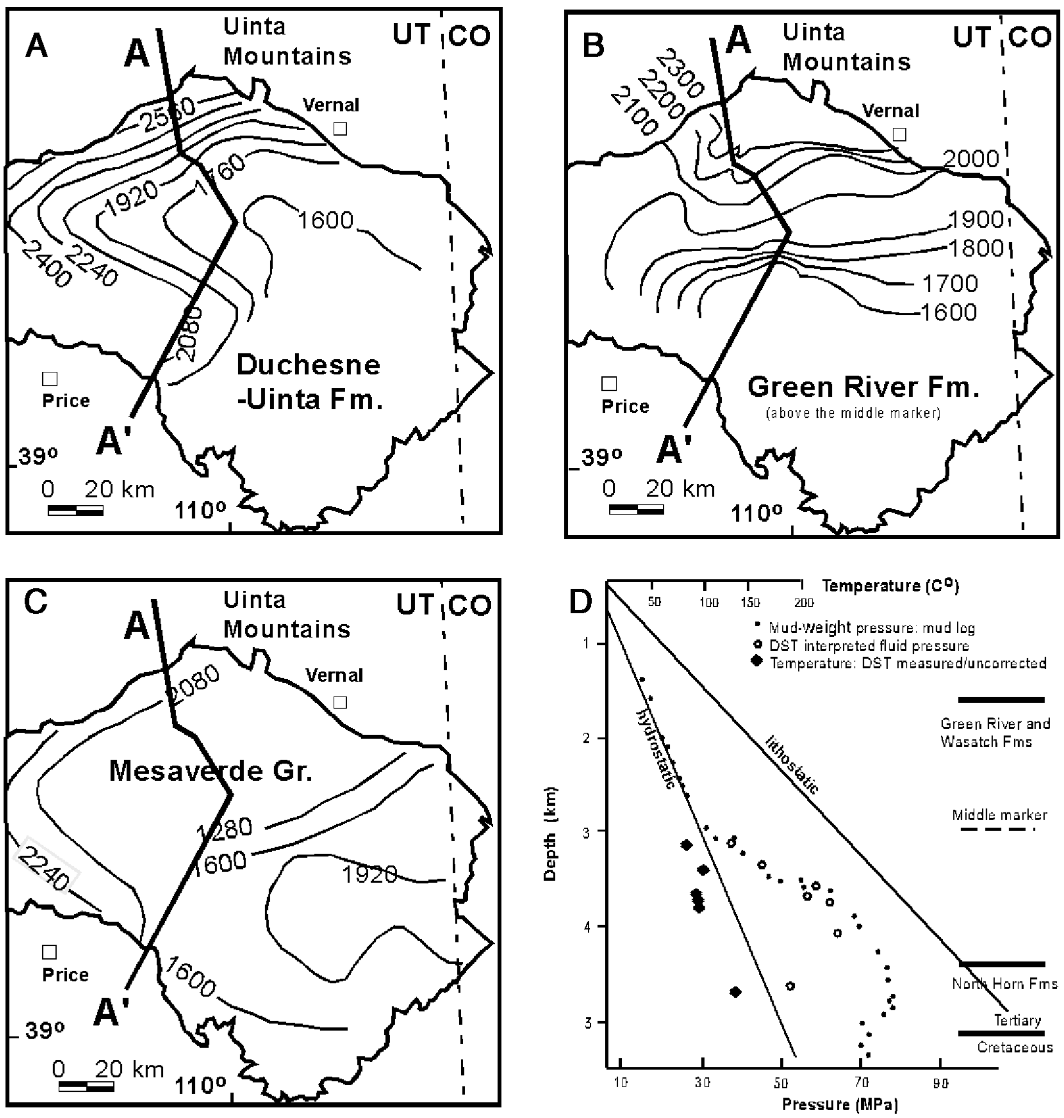


Figure 8. The observed hydraulic heads (in m) within the shallow Duchesne-Uinta Formations (A), the upper Green River Formation (B), and the deep Mesaverde Group (C) of the Uinta Basin (Bredeheoft et al., 1994, Ground Water Atlas of the United States, 1995). Also shown are the downhole temperature and pressure conditions representative of the lower Green River Formation at the Altamont-Bluebell field (D) (after Spencer, 1987).

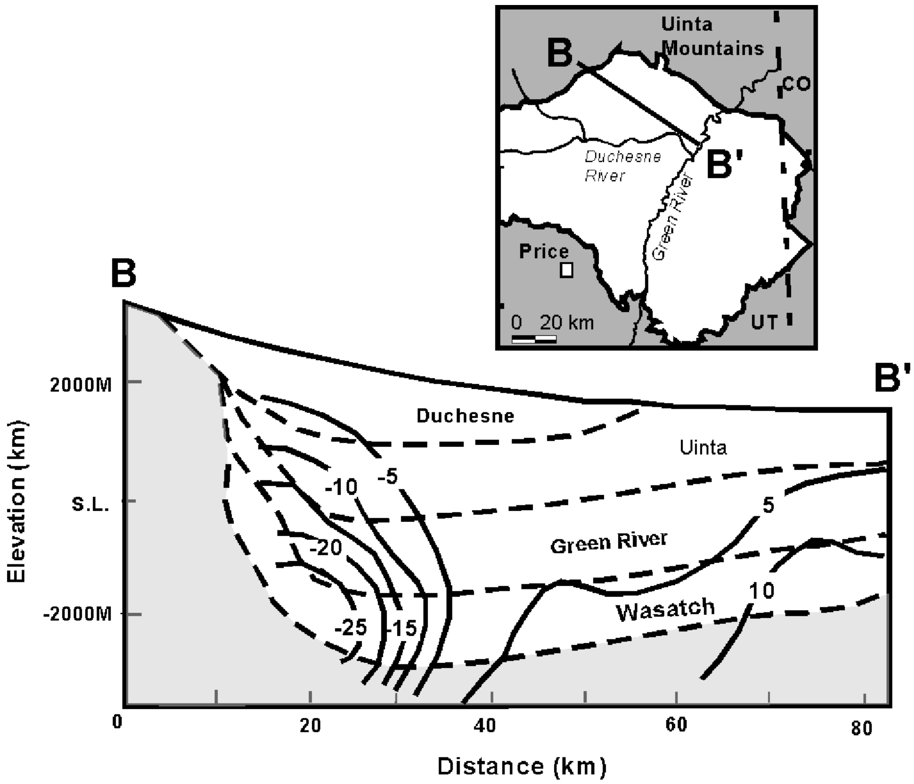
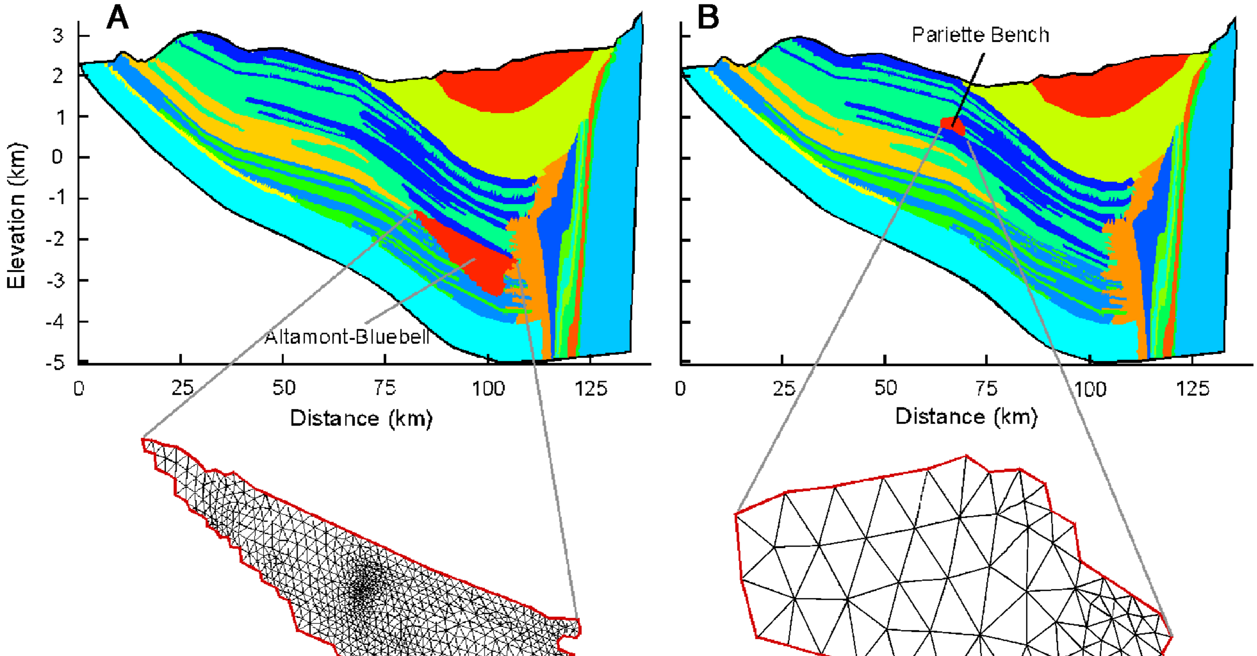
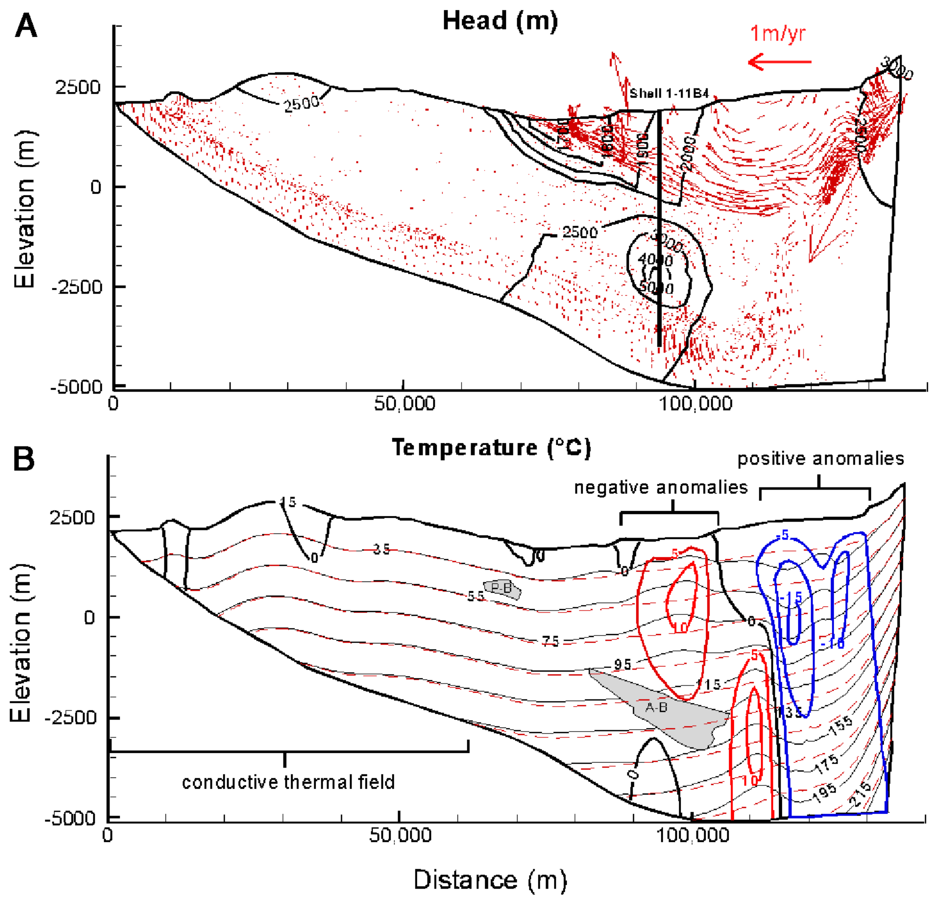


Figure 9. A contour map of the inferred temperature anomalies - deviation from the conductive temperatures (in °C) in the Uinta Basin (after Willett and Chapman, (1989).



	nnode	nelem
basin	14544	28768
A-B	767	1404
P-B	76	118

Figure 10. The numerical representations of the cross-sectional transect in the Uinta Basin (color coded to represent the different stratigraphies as well as the locations of the oil reservoirs simulated. (A) The location of the Altamont-Bluebell oil reservoir (A-B) and the numerical grid used to represent it. (B) The location of the Pariette Bench oil reservoir (P-B) and the grid used to represent it. The location of this cross section in the Uinta Basin is shown in Figure 1.



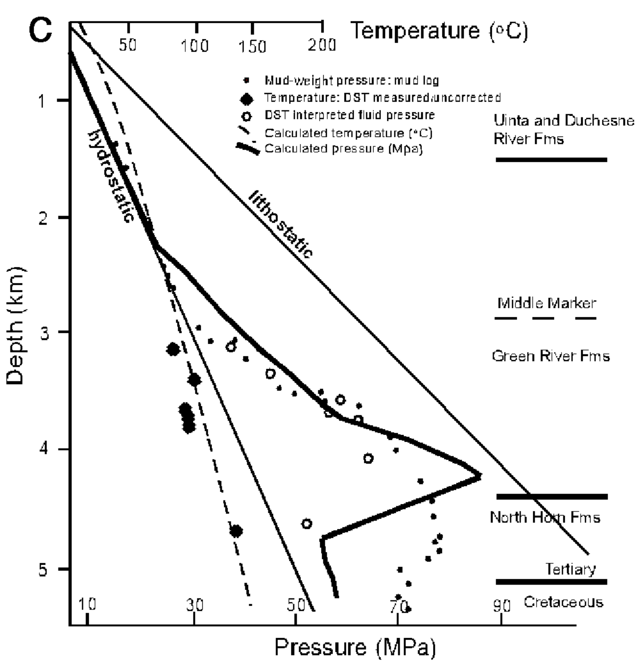


Figure 11 (A) The calibrated head (m) and ground-water velocities (m/yr) in the basin. Location of Shell 1-11 B4 Brotherson well is shown by a bold line. (B) The calibrated temperature (°C) in the basin. Location of the oil fields are indicated. A-B: Altamont-Bluebell field; P-B: Pariette Bench field. The computed temperatures for the Altamont-Bluebell and the Pariette Bench fields fall within the observed temperature ranges at these fields which varies from 80 to 130 °C in A-B and 45 to 60 °C in P-B. An conductive thermal field is also shown which can exist in a static groundwater system. The difference between the advective and conductive field is the temperature anomalies which are positive near the recharge area and negative near the discharge area. The location and the magnitude of the temperature anomalies are also consistent with the observed conditions. (C) The calibrated downhole temperature and pressure profiles in Shell 1-11 B4 well in the A-B field. Observed data (dots) are plotted for comparison.

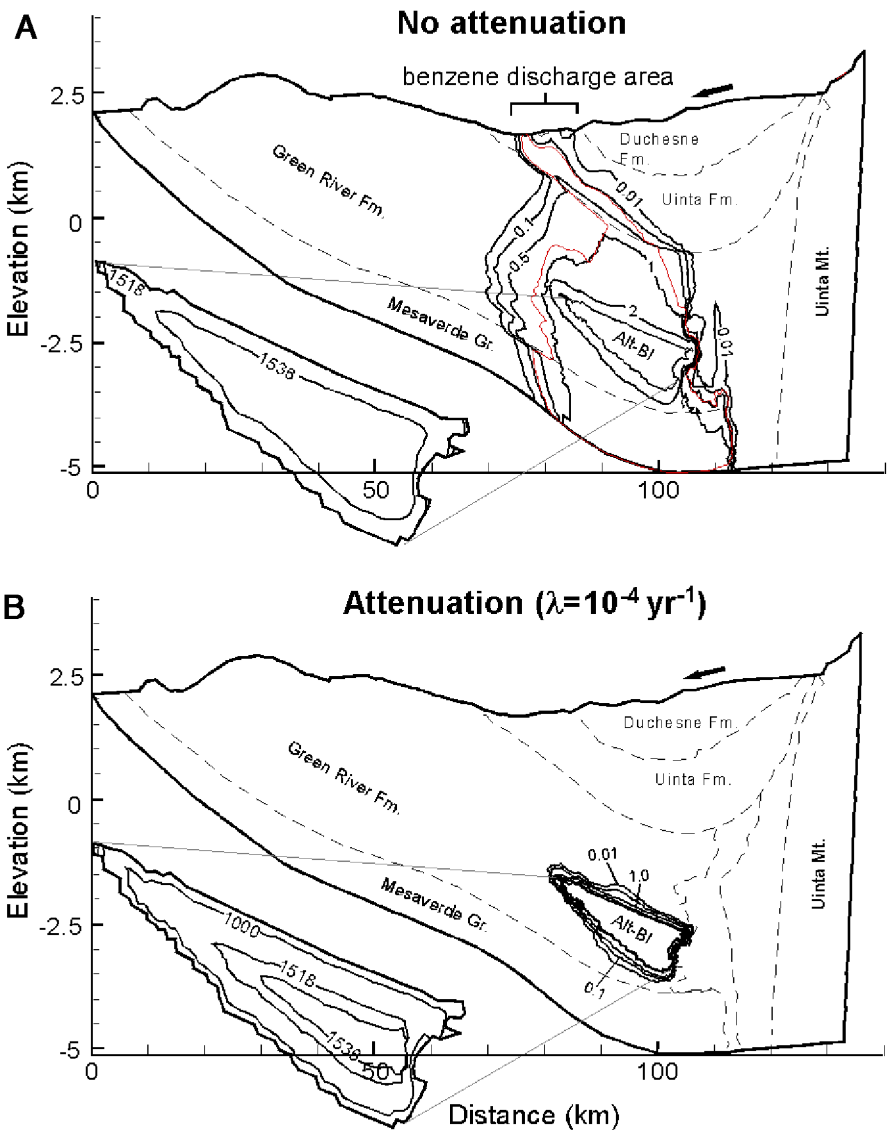


Figure 12. (A) The calculated benzene concentrations (ppm) in the Uinta Basin and in the Altamont-Bluebell oil reservoir at the end of 5 million years, with no attenuation. The red lines is the 0.01 concentration contour at 1 million years. (B) The calculated benzene concentrations (ppm) in the basin and the oil reservoir when attenuation was represented. The arrow indicates the general direction of the groundwater flow within the upper flow system of the Duchesne-Uinta Formations. Dashed lines indicate the boundaries between the major stratigraphic units.